**ภาคผนวก ก**

**การวิเคราะห์ข้อมูล**

**ตารางภาคผนวกที่ 1** คำนวณพลังงานการยึดจับและพลังงานการดูดซับ

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| ระบบ | SWCNT หรือ  TM-SWCNT | โลหะ หรือ แก๊ส | TM-หรือ gas/ TM-SWCNT | ∆*E*ads  (amu.) | ∆*E*ads  (kcal/mol) |
| Sc-SWCNT | -3402.809 | -46.363 | -3449.432 | -0.260 | -163.377 |
| Ti-SWCNT | -3402.809 | -57.908 | -3461.049 | -0.332 | -208.058 |
| V-SWCNT | -3402.809 | -71.158 | -3474.277 | -0.310 | -194.395 |
| Cr-SWCNT | -3402.809 | -85.815 | -3489.207 | -0.583 | -365.867 |
| Mn-SWCNT | -3402.809 | -103.752 | -3506.856 | -0.294 | -184.726 |
| Y-SWCNT | -3402.809 | -37.848 | -3440.909 | -0.252 | -157.921 |
| Zr-SWCNT | -3402.809 | -46.383 | -3449.537 | -0.345 | -216.481 |
| Nb-SWCNT | -3402.809 | -56.104 | -3459.267 | -0.354 | -222.190 |
| Mo-SWCNT | -3402.809 | -67.249 | -3470.462 | -0.404 | -253.449 |
| Tc-SWCNT | -3402.809 | -79.835 | -3483.037 | -0.393 | -246.755 |
| NH3/SWCNT | -3441.157 | -56.548 | -3497.706 | -0.001 | -0.7213 |
| PH3/SWCNT | -3441.157 | -8.270 | -3449.428 | -0.001 | -0.5148 |
| AsH3/SWCNT | -3441.157 | -7.834 | -3448.992 | -0.001 | -0.340 |
| NH3/Sc-SWCNT | -3449.432 | -56.548 | -3506.028 | -0.048 | -29.808 |
| PH3/Sc-SWCNT | -3449.432 | -8.270 | -3457.725 | -0.023 | -14.473 |
| AsH3/Sc-SWCNT | -3449.432 | -7.834 | -3457.347 | -0.080 | -50.320 |
| NH3/Ti-SWCNT | -3461.049 | -56.548 | -3517.655 | -0.058 | -36.236 |
| PH3/Ti-SWCNT | -3461.049 | -8.270 | -3469.349 | -0.030 | -18.627 |
| AsH3/Ti-SWCNT | -3461.049 | -7.834 | -3468.969 | -0.086 | -54.192 |
| NH3/V-SWCNT | -3474.277 | -56.548 | -3530.880 | -0.054 | -34.142 |
| PH3/V-SWCNT | -3474.277 | -8.270 | -3482.585 | -0.039 | -24.159 |
| AsH3/V-SWCNT | -3474.277 | -7.834 | -3482.206 | -0.095 | -59.754 |
| NH3/Cr-SWCNT | -3489.207 | -56.548 | -3545.815 | -0.059 | -37.163 |
| PH3/Cr-SWCNT | -3489.207 | -8.270 | -3497.513 | -0.036 | -22.562 |
| AsH3/Cr-SWCNT | -3489.207 | -7.834 | -3497.134 | -0.092 | -58.291 |

**ตารางภาคผนวกที่ 2** คำนวณแถบพลังงาน

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| ระบบ | *E*HOMO(au) | *E*HOMO(eV) | *E*LUMO(au) | *E*LUMO(eV) | *E*gap(eV) | ∆*E*gap(eV) |
| SWCNT | -0.162 | -4.408 | -0.121 | -3.293 | 1.116 | - |
| Sc-SWCNT | -0.147 | -4.000 | -0.104 | -2.830 | 1.170 | -0.054 |
| Ti-SWCNT | -0.152 | -4.136 | -0.112 | -3.048 | 1.088 | 0.027 |
| V-SWCNT | -0.166 | -4.517 | -0.117 | -3.184 | 1.333 | -0.218 |
| Cr-SWCNT | -0.160 | -4.354 | -0.118 | -3.211 | 1.143 | -0.027 |
| Mn-SWCNT | -0.145 | -3.946 | -0.102 | -2.776 | 1.170 | -0.054 |
| Y-SWCNT | -0.145 | -3.946 | -0.102 | -2.776 | 1.170 | -0.054 |
| Zr-SWCNT | -0.149 | -4.055 | -0.110 | -2.993 | 1.061 | 0.054 |
| Nb-SWCNT | -0.154 | -4.191 | -0.122 | -3.320 | 0.871 | 0.245 |
| Mo-SWCNT | -0.158 | -4.300 | -0.124 | -3.374 | 0.925 | 0.190 |
| Tc-SWCNT | -0.164 | -4.463 | -0.116 | -3.157 | 1.306 | -0.190 |
| NH3/SWCNT | -0.163 | -4.436 | -0.122 | -3.320 | 1.116 | - |
| NH3/Cr-SWCNT | -0.151 | -4.109 | -0.110 | -2.993 | 1.116 | 0.000 |
| NH3/Sc-SWCNT | -0.140 | -3.810 | -0.097 | -2.640 | 1.170 | -0.054 |
| NH3/Ti-SWCNT | -0.144 | -3.919 | -0.104 | -2.830 | 1.088 | 0.027 |
| NH3/V-SWCNT | -0.146 | -3.973 | -0.108 | -2.940 | 1.034 | 0.082 |
| PH3/SWCNT | -0.163 | -4.436 | -0.122 | -3.320 | 1.116 | - |
| PH3/Cr-SWCNT | -0.156 | -4.245 | -0.113 | -3.075 | 1.170 | -0.054 |
| PH3/Sc-SWCNT | -0.142 | -3.864 | -0.099 | -2.694 | 1.170 | -0.054 |
| PH3/Ti-SWCNT | -0.146 | -3.973 | -0.106 | -2.885 | 1.088 | 0.027 |
| PH3/V-SWCNT | -0.146 | -3.973 | -0.104 | -2.830 | 1.143 | -0.027 |
| AsH3/SWCNT | -0.162 | -4.408 | -0.120 | -3.265 | 1.143 | - |
| AsH3/Cr-SWCNT | -0.157 | -4.272 | -0.114 | -3.102 | 1.170 | -0.027 |
| AsH3/Sc-SWCNT | -0.143 | -3.891 | -0.099 | -2.694 | 1.197 | -0.054 |
| AsH3/Ti-SWCNT | -0.147 | -4.000 | -0.107 | -2.912 | 1.088 | 0.054 |
| AsH3/V-SWCNT | -0.147 | -4.000 | -0.105 | -2.857 | 1.143 | 0.000 |